Strong coupling resistivity in the Kondo model.

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By applying methods of integrable quantum field theory to the Kondo problem, we develop a systematic perturbation expansion near the IR (strong coupling) fixed point. This requires the knowledge of an infinity of irrelevant operators and their couplings, which we all determine exactly. A low temperature expansion (ie all the corrections to Fermi liquid theory) of the resistivity then follows, extending for instance the well known Nozières T^2 result in the exactly screened case to arbitrary order. The example of the ordinary Kondo model is worked out in details: we determine ρ up to order T^6, and compare the result with available numerical data.

Theoretical progress in the understanding of the Kondo model over the last twenty years has been remarkable (see [1] for a review). Most of the interest has focussed on the strong coupling fixed point, where non perturbative techniques like the numerical renormalization group, the Bethe ansatz [2] and conformal field theory [3] have provided many powerful results. Yet, the basic quantity that gave rise to the discovery of the Kondo physics itself, the resistivity ρ, has remained strangely resilient to analytical understanding : although its behaviour is well understood, based on various numerical renormalization or approximation methods, essentially no exact results have been obtained for it - for instance, it cannot be computed by the Bethe ansatz, in contrast with the specific heat, or the magnetic susceptibility. A notable exception to this state of affairs is the result of Nozières [4] for the ordinary Kondo problem, which gives the exact first order correction to the resistivity near the strong coupling (IR) fixed point (see below). This result has since been generalized to the case of several channels and higher spins [1].

It is important here to emphasize that studying the vicinity of the strong coupling fixed point is a subtle challenge. In the case of the weak coupling (UV) fixed point, one at least knows the effective hamiltonian, up to irrelevant terms, so the universal properties at high temperature can in principle be accessed perturbatively. As is well known, this perturbation breaks down at some point. A natural idea to study the low temperature properties is thus to perturb around the other, strong coupling fixed point. In that case however, all the operators are irrelevant. The leading irrelevant operator is usually the only one kept in the computations: it is this operator that gives rise to the Fermi liquid or Nozières result in the exactly screened case, or the results of Affleck and Ludwig in the overscreened case [5]. To go beyond first order, one however needs to know the *next* irrelevant operators, together with their coupling constants. This is a difficult problem, that cannot be answered by qualitative arguments. As we will see below, even the form of the operators is not obvious, and requires a complicated adjustment. The only way to determine precisely the hamiltonian near the IR fixed point is to use, somehow, the fact that it is the "large coupling limit" of the known hamiltonian near the UV fixed point. How to do that in practice however was a largely open problem up to now. A few years ago, Hewson [6] introduced a "renormalized perturbation theory" that should in principle answer the question : in practice however, the method seems very hard to implement, and we are not aware of any quantitative correction to the Fermi liquid behaviour obtained in that way.

The main result of this paper is the exact determination of the hamiltonian near the IR fixed point to *all* orders. It is then a purely technical matter to determine the corrections to the resistivity. We carry them out to order T^6 in the ordinary Kondo problem, and compare with existing numerical data.

Let us now define the problem in more details. We follow closely the notations of [5]. We take as the starting hamiltonian

$$\mathcal{H} = \sum_{k,\mu} \psi_k^{\dagger\mu}\psi_{k\mu}\epsilon(k) + \lambda\vec{S}\cdot\sum_{k,k'}\psi_k^{\dagger\mu}\frac{\vec{\sigma}_\mu^\nu}{2}\psi_{k'\nu}, \qquad (1)$$

with μ the spin label. Assuming that the impurities are dilute enough so we can restrict to the case of only one impurity, we decompose as usual the fermionic field on spherical harmonics. Only the s-wave interacts with the impurity and, at low energies, its field operator takes the form

$$\Psi(\vec{r}) = \frac{1}{2\sqrt{2}i\pi r}[e^{ip_F r}\psi_R(r) - e^{-ip_F r}\psi_L(r)], \qquad (2)$$

with the proper linearisation of the dispersion relation in that limit, ie $\epsilon_p \simeq v_F(p-p_F) \equiv v_F p'$. The resistivity can be obtained by using the Kubo formula for the conductivity, following [5]

$$\frac{1}{\rho(T)} = \sigma(T) = 2\frac{e^2}{3m^2}\int\frac{d^3\vec{p}}{(2\pi)^3}\left[-\frac{dn}{d\epsilon_k}\right]\vec{p}\cdot\vec{p}\,\tau(\epsilon_p), \quad (3)$$

with the single particle lifetime defined by $1/\tau = -2\mathrm{Im}\Sigma^R$. Σ^R, the retarded self-energy, is obtained from the three-dimensional Green's function which in turns follows from the one-dimensional s-wave contributions [5]

$$G(\omega_M,\vec{r}_1,\vec{r}_2)-G^0(\omega_M,\vec{r}_1-\vec{r}_2)= \frac{-1}{8\pi^2 r_1 r_2}\Big[e^{-ik_F(r_1+r_2)}(G^{(1D)}_{LR}-G^{0(1D)}_{LR}) +e^{ik_F(r_1+r_2)}(G^{(1D)}_{RL}-G^{0(1D)}_{RL})\Big]. \quad (4)$$

Here the superscript 0 means that the Green's function is evaluated with respect to the non-interacting UV fixed point where $\psi_R(0)=\psi_L(0)$ as a consequence of the spherical harmonic decomposition. Eq (4) can be rewritten as

$$G(\omega_M,\vec{r}_1,\vec{r}_2)-G^0(\omega_M,\vec{r}_1-\vec{r}_2)= G^0(\omega_M,\vec{r}_1)T(\omega_M)G^0(\omega_M,-\vec{r}_2). \quad (5)$$

One can then sum over the dilute array of random impurities, restoring translation invariance. The summation over multi-impurity terms leads to the self energy $\Sigma(\omega_M)=n_i T(\omega_M)$, to first order in n_i, the impurity density. As usual, impurity-impurity interactions are neglected, and the following results should be reliable for dilute impurities (see [5], [7] for more discussion on that point). The retarded self-energy is found by analytical continuation, $i\omega_M\to\omega+i0$. It leads to the single particle lifetime, and thus to the resistivity using (3).

It is thus clear, as stressed in [5], that the RL and LR components of the $1D$ Green's functions are the only necessary ingredients to compute the resistivity, and we will concentrate on these in the following. At the IR fixed point, the spin is completely screened and the interaction with the impurity amounts to a phase shift, which in the one-channel case is simply encoded in the boundary conditions $\psi_R(0)=-\psi_L(0)$: this leads to the result $\Sigma^R(\omega)=-\frac{in_i}{\pi\nu}$, where ν is the density of states per spin.

To proceed, we bosonize the one dimensional theory, setting $\psi_{R/L,\mu}=\exp\left(\pm i\sqrt{4\pi}\phi_\mu\right)$ (our normalization for the fermions follows [5] anddoes not contain the usual factors of 2π). The spin and charge degrees of freedom then completely decouple from each other and, using spin and charge fields

$$\phi_s=\frac{1}{\sqrt{2}}(\phi_\uparrow-\phi_\downarrow),\ \phi_c=\frac{1}{\sqrt{2}}(\phi_\uparrow+\phi_\downarrow), \quad (6)$$

the interaction only involves the spin field, with hamiltonian

$$\mathcal{H}_{UV}=\mathcal{H}^*+\lambda[S_- e^{i\sqrt{2\pi}\phi_s(0)}+c.c.] \quad (7)$$

where right and left movers have been combined in one field, and $\mathcal{H}^*=\frac{1}{2}\int_{-\infty}^0 dx[(\partial_x\phi_s)^2+\Pi_s^2]$ is a free boson hamiltonian. To write (7) we have performed an additional canonical transformation to get rid of the S_z terms. In the usual approximation where the band structure does not mix up spin and charge, the RG flow is completely controlled by the spin sector.

The hamiltonian (7) defines an integrable boundary quantum field theory [8]. Although much progress has been made in computing physical properties by using integrability [2], including some correlators [9], the resistivity so far has not been accessible. The two reasons for that are: the divergence of the form factors expansion when the perturbing operator has dimension 1 as in (7), and the fact that the resistivity is really a three dimensional quantity, following in a very non trivial way only from the one dimensional computations.

Our strategy here will be to use integrability to determine the exact form of the IR hamiltonian. Once this is obtained, we will be able to do perturbation theory near the IR fixed point: short of a Bethe ansatz determination of the resistivity, this seems the most powerful approach at the present time.

We write

$$\mathcal{H}_{IR}\equiv\mathcal{H}^*+\delta\mathcal{H}=\mathcal{H}^*+\sum_{k=0}^{\infty}u_{2k+1}\mathcal{O}_{2k+2}(0), \quad (8)$$

where the coupling constants u and operators $\mathcal{O}$ have to be determined. In (8), $\mathcal{H}^*$ is still a fre boson hamiltonian. However, due to the modified boundary condition $\psi_L=-\psi_R$ at the IR fixed point, we have $\phi_L(0)=\phi_R(0)+i\sqrt{\frac{\pi}{4}}$.

It is fair to say at this stage that the determination of (8) follows implicitely from the works of Bazhanov et al. [10]. We present here a much more direct, and generalizable, argument. The main idea is the following: we first restrict to $T=0$, and we switch the description from "open string channel" as in (7) (where imaginary time is in the y direction), to the "closed string channel", where imaginary time is now along x. In that case, the theory is described by a free boson hamiltonian, and all the interactions are encoded in a boundary state $|B\rangle$. The latter takes a simple form [8] because of integrability:

$$|B\rangle\propto\exp\left[\int\frac{d\beta}{2\pi}K(\beta-\log T_B)\sum_{\epsilon=\pm}Z^*_{L\epsilon}(\beta)Z^*_{R\epsilon}(\beta)\right]|0\rangle. \quad (9)$$

Here, $|0\rangle$ is the ground state of the theory in the open string channel, T_B is proportional to the Kondo temperature (we discuss their exact relation below), the Z^*_ϵ are creation operators for the kinks and antikinks of the massless sine-Gordon theory [11] - that is, the basis diagonalising the interaction. β is the rapidity of the massless kinks, satisfying $e=\pm p=e^\beta$ for right (resp. left) movers. We do not need the precise way in which the kinks and antikinks behave to explain the argument: it suffices to say that their scattering in the bulk is factorized, and that, in the open channel picture, they bounce on the boundary in a factorized way too, with a reflection matrix that is simply related with K. Here, $K(\beta)=-i\tanh\frac{\beta}{2}$. To proceed, let us now expand $|B\rangle$ around the IR fixed point, ie for T_B large. We get

$$|B\rangle=\exp\left[-\sum_{k=0}^{\infty}\frac{1}{(2k+1)T_B^{2k+1}}\widehat{\mathcal{I}}_{2k+1}\right]|B\rangle^* \quad (10)$$

where $|B\rangle^*$ is the IR boundary state and the $\widehat{\mathcal{I}}_{2k+1}$ are the standard conserved quantities of the theory: they act diagonally on the multiparticles states with eigenvalues

$$\widehat{\mathcal{I}}_{2k+1}|\beta_1...\beta_n\rangle_{C_1,\epsilon_1\cdots} = \left(\sum_i e^{(2k+1)\beta_i}\right)|\beta_1...\beta_n\rangle_{C_1,\epsilon_1,\cdots}, \tag{11}$$

with C_i the chirality. By comparing with the general formula $|B\rangle = \mathcal{P}\exp[-\int dy\delta\mathcal{H}]|B\rangle^*$, where $\mathcal{P}$ exp is the y-path ordered exponential, we can identify the hamiltonian. The last step to do so is to reexpress the $\widehat{\mathcal{I}}_{2k+1}$ in terms of (integrals of) local operators of the theory. This is easy to do, using the condition that these operators must be mutually commuting (how to find the proper normalization will be discussed in a subsequent publication [12]). After a Wick rotation to go back to the open string channel, the final result is

$$u_{2k+1} = \frac{1}{\pi^k(k+\frac{1}{2})(k+1)!}T_B^{-(2k+1)} \tag{12}$$

together with the form of the operators [13]

$$\begin{aligned}
\mathcal{O}_2 &= -\frac{1}{4\pi}\left(T_{ww}+T_{\bar{w}\bar{w}}\right)\\
\mathcal{O}_4 &= \frac{1}{4\pi}\left(:T_{ww}^2:+w\to\bar{w}\right)\\
\mathcal{O}_6 &= -\frac{1}{4\pi}\left(:T_{ww}^3:+\frac{1}{4}:T_{ww}\partial_w^2T_{ww}:+w\to\bar{w}\right)\\
&\cdots
\end{aligned} \tag{13}$$

Here, the basic object is the stress energy tensor $T_{ww} = -2\pi:\left(\partial_w\phi_s\right)^2:(w=-y+ix)$; it is the leading irrelevant operator near the IR fixed point, a result well known from previous work [5]. Up to an overall normalization, there is no ambiguity it: it is the only operator of dimension 2, up to total derivatives. This is hardly true however for the next to leading irrelevant operators: they involve very particular combinations of powers of derivatives of ϕ_s, and could not have been guessed on general grounds, without using the constraint of integrability. The case of $\mathcal{O}_2$ is an exception, where, after refermionization, one finds

$$\mathcal{O}_2 \propto 2:\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow^\dagger\psi_\downarrow: -i:\psi_\uparrow^\dagger\partial_y\psi_\uparrow: -i:\psi_\downarrow^\dagger\partial_y\psi_\downarrow: \tag{14}$$

It is proportionnal to $\vec{J}(0)\cdot\vec{J}(0)$ (up to total derivatives), with $\vec{J}$ the spin current [14].

Notice that the more irrelevant operators in (8) come with prefactors that are inverse powers of the Kondo temperature: due to this rescaling, they *cannot* be neglected, and a perturbation expansion to n^{th} non trivial order near the IR fixed point requires the knowledge of the terms in (8) up to $k=n$. This is in contrast with the situation near the UV fixed point, where the coefficients of the irrelevant operators are dictated by the microscopic theory, and usually all of the same order, so only the leading relevant one remains in the universal scaling regime. Here, the vicinity of the IR fixed point is fully determined by the constraint that it is the large coupling limit of the UV one, and this is what produces the fine tuning.

It is important to emphasize that our IR hamiltonian makes sense only within a well defined regularization scheme. Since all this is based on the formalism of integrable quantum field theories where no cut-off ever appears, we have to regularize our integrals by contour splitting, as explained below.

Let us now discuss how to compute the resistivity. The first operator perturbing the fixed point is $:\left(\partial_y\phi_s\right)^2:$, the energy momentum tensor. To order $\frac{1}{T_B}$ for instance, the correction to the RL 1D Green's function for the up-spin electrons reads

$$\begin{aligned}
\delta G_{RL}^{(1)} = \frac{2}{T_B}\int_{-\beta/2}^{\beta/2}dy e^{i\omega_M y}\int_{-\beta/2}^{\beta/2}dy' \\
\langle e^{i\sqrt{2\pi}(\phi_c+\phi_s)}:\left(\partial_{y'}\phi_s\right)^2:e^{-i\sqrt{2\pi}(\phi_c+\phi_c)}\rangle^*,
\end{aligned} \tag{15}$$

where the propagators have to be evaluated with the IR fixed point hamiltonian. The integrals in (15) can be quickly evaluated by closing the contour in the complex plane using the periodicity of the integrand. The result is simply

$$-\frac{2i\pi}{T_B}e^{-\omega_M(r_1+r_2)}\omega_M\epsilon(\omega_M). \tag{16}$$

Since this term is purely imaginary, it contributes a real term to the self energy, and does not affect the resistivity. At order $\frac{1}{T_B^2}$, $\mathcal{O}_2$ is still the only operator to contribute. The integrals now present divergences where two of the $\mathcal{O}_2$ operators come close. These divergences are simply regulated by shifting one of the contours slighlty off in the imaginary direction. One finds finally

$$\Sigma^R(\omega) = -\frac{in_i}{2\pi\nu}\left[2+i\frac{\omega}{T_B}-\frac{1}{4T_B^2}(3\omega^2+(\pi T)^2)\right], \tag{17}$$

in agreement with [5].

We now extend the computation beyond this order. At order $1/T_B^3$, it becomes necessary to include, in addition to the energy momentum tensor, the higher conserved operator $\mathcal{O}_4$. In manipulating $\mathcal{O}_4$, one has to be very careful that it is not a primary field: its correlation functions on the cylinder (ie at finite temperature) contain anomalous terms, that can be computed from general conformal field theory arguments (for instance, one finds $:T_{ww}^2:=4\pi^2:\left(\partial_w\phi_s\right)^4:-2\pi:\partial_w\phi_s\partial_w^3\phi_s:-2\pi^3T^2:\left(\partial\phi_s\right)^2:+\frac{3\pi^4T^4}{20}$). As before, this order does not contribute to the resistivity. At order $\frac{1}{T_B^4}$, $\mathcal{O}_2$ and $\mathcal{O}_4$ are still the only operators that contribute, and we find

$$\Sigma^R(\omega) = -\frac{in_i}{2\pi\nu}\Big[2 + i\frac{\omega}{T_B} - \frac{1}{4T_B^2}\left(3\omega^2 + (\pi T)^2\right) - i\left(\frac{5}{12} + \frac{3}{24\pi}\right)\left(\frac{\omega}{T_B}\right)^3 - i\left(\frac{1}{4} + \frac{1}{8\pi}\right)\frac{\omega}{T_B}\left(\frac{\pi T}{T_B}\right)^2 + \left(\frac{35}{192} + \frac{7}{32\pi}\right)\left(\frac{\omega}{T_B}\right)^4 + \left(\frac{19}{96} + \frac{5}{16\pi}\right)\left(\frac{\pi T}{T_B}\right)^2\left(\frac{\omega}{T_B}\right)^2 + \left(\frac{11}{192} + \frac{3}{32\pi}\right)\left(\frac{\pi T}{T_B}\right)^4\Big] \quad (18)$$

In these computations, very strong short distance divergences are of course generally encountered (there are no large distance divergences due to the temperature T that acts as a cut-off). To regularize them, as for the second order case, we slightly move the contours off one another, and use the residue theorem to evaluate the resulting integrals. The commutativity of all the $\widehat{\mathcal{I}}_{2k+1}$ means that the short distance expansions of the operators $\mathcal{O}_{2k+2}$ have simple poles whose residues are total derivatives: this ensures that the final result does not depend on the order in which this regularization is implemented.

We have carried out the computation further to fifth and sixth order. The expression for the self energy is too bulky to be given here, but, by using the Kubo formula as in [5], it leads to our main result for the resistivity

$$\rho(T) = \frac{3n_i}{\pi(ev_F\nu)^2}\Big[1 - \frac{1}{4}(\frac{\pi T}{T_B})^2 + \left(\frac{13}{240} + \frac{3}{20\pi}\right)(\frac{\pi T}{T_B})^4 + \left(\frac{47}{10080} - \frac{1}{8\pi} - \frac{53}{336\pi^2}\right)(\frac{\pi T}{T_B})^6 + \cdots\Big] \quad (19)$$

where ν is the density of states per spin. The order T^2 allows us to quickly match normalizations with other works - see for instance appendix K in the book by Hewson [1] and we find $T_B = \frac{2T_K}{\pi w}$, T_K the usual Kondo temperature, $w = 0.41071$ the Wilson number (compared to the review by Andrei et al. [2], $T_B = 2T_0$). The orders T^4 and T^6 in (19) are new.

In general theories, one expects IR expansions to be only asymptotic. However, for integrable quantum impurity problems, these expansions often turn out to be convergent. Assessing the status of the T^2 expansion of the resistivity is a bit difficult: based on our numerical values, it seems to converge, but with a disappointingly small radius of convergence. That the radius is so small presumably explains why estimates of T_K from numerical or experimental data on the resistivity often differ significantly from estimates based eg on the susceptibility (where convergence is good, as is easily checked on the Bethe ansatz results). The comparison of our formula (19) with the result of numerical renormalisation group methods carried out by Costi et al. [15] on the Anderson model is shown on the following figure. Clearly more orders would be needed to go beyond $T/T_B \approx .2$. Padé approximants however turn out to be quite stable, and agree well with the data up to $T/T_B \approx 1$, which is well in the crossover regime. We thus believe that our results present a rather complete analytical understanding of the strong coupling resistivity.

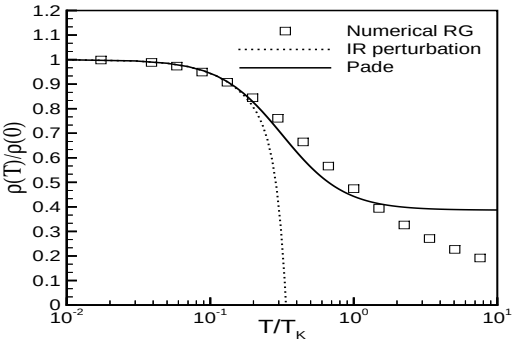

FIG. 1. Comparison of IR perturbation theory with numerical RG results.

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